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Bis{2-[3-(cyclohexylaminio)propyliminomethyl]-4-nitrophenolato}dimethanolnickel(II) dinitrate dihydrate

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Key indicators

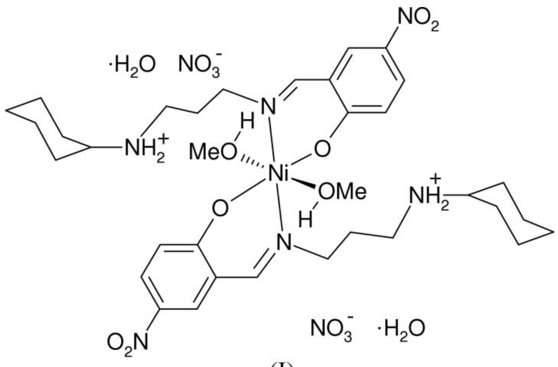
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.107
Data-to-parameter ratio = 18.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title complex, $[Ni(C_{16}H_{23}N_3O_3)_2(CH_4O)_2](NO_3)_2\cdot 2H_2O$, a mononuclear centrosymmetric nickel(II) compound, the Ni^{II} atom is six-coordinated in an octahedral geometry by two imine N and two phenolate O atoms from two Schiff base ligands, and by two O atoms from two coordinated MeOH molecules. In the crystal structure, the molecules are linked through intermolecular O—H···O, N—H···O and N—H···N type hydrogen bonds, forming layers parallel to the *bc* plane.

Comment

Transition metal complexes containing Schiff base ligands have been of great interest for many years (Yamada, 1999). These complexes play an important role in the coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Lacroix, 1996; Goswami & Eichhorn, 1999; Rybak-Akimova *et al.*, 1998). Studying the variety of products in the self-assembly processes between labile metal ions and flexible multidentate ligands is an interesting topic in supramolecular chemistry (You, 2005*a*,*b*,*c*,*d*,*e*,*f*; You & Zhu, 2005). Here we report the title new nickel(II) complex, (I).



(I)

Complex (I) is a mononuclear centrosymmetric nickel(II) compound, with the Ni^{II} atom lying on the inversion center (Fig. 1). The complex consists of a mononuclear $[Ni(C_{16}H_{23}N_3O_3)_2(MeOH)_2]^{2+}$ cation, two uncoordinated nitrate anions, and two uncoordinated water molecules. In the cation, the Ni^{II} atom is six-coordinated in an octahedral geometry by two imine N and two phenolate O atoms from two Schiff base ligands, and by two O atoms from two coordinated MeOH molecules. The *trans* angles at the Ni^{II} center are exactly 180° (Table 1) due to the crystallographic symmetry. All other angles subtended at the Ni^{II} atoms are close to 90°, varying from 86.32 (5) to 93.68 (5)°. The dihedral angle between the O2—N1—O3 plane and the C1–C6 benzene ring is 6.2 (2)°. As

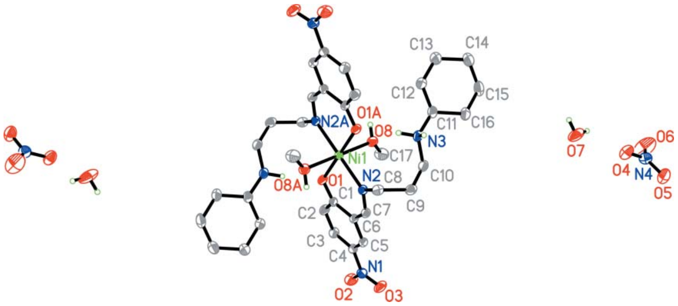


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. C-bound H atoms have been omitted for clarity. Atoms labelled with the suffix A are at the symmetry position $(1 - x, 1 - y, 1 - z)$.

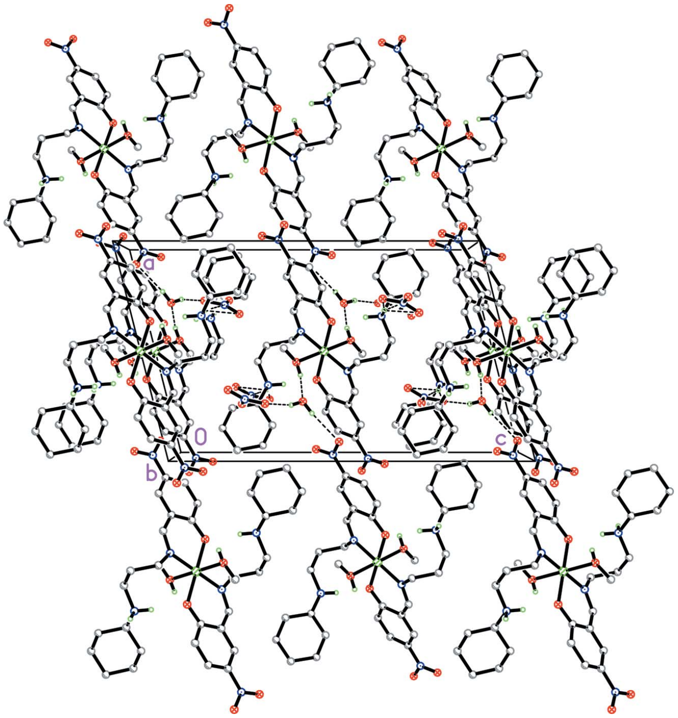


Figure 2
The crystal packing of (I), viewed along the b axis. C-bound H atoms have been omitted for clarity. Dashed lines indicate hydrogen bonds.

expected, the cyclohexyl groups in the complex adopt chair conformations to minimize steric effects.

In the crystal structure, molecules are linked through intermolecular O—H···O, N—H···N and N—H···O hydrogen bonds (Table 2), forming layers parallel to the *ab* plane (Fig. 2).

Experimental

N-Cyclohexyl-1,3-diaminopropane (0.1 mmol, 15.6 mg) and 5-nitrosalicylaldehyde (0.1 mmol, 16.7 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. To this solution was added an aqueous solution (5 ml) of $Ni(NO_3)\cdot6H_2O$ (0.1 mmol, 29.1 mg), with stirring. The resulting mixture was stirred for another 10 min at room temperature and filtered. After keeping the filtrate in air for 7 d, green block-shaped crystals were formed.

Crystal data

$[Ni(C_{16}H_{23}N_3O_3)_2(CH_4O)_2]$-
$(NO_3)_2\cdot2H_2O$
$M_r = 893.59$
Monoclinic, $P2_1/c$
$a = 12.428$ (1) Å
$b = 8.755$ (1) Å
$c = 20.048$ (1) Å
$\beta = 104.20$ (1)°
$V = 2114.7$ (3) Å^3
$Z = 2$

$D_x = 1.403$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7814 reflections
$\theta = 2.4$–26.3°
$\mu = 0.54$ mm^{-1}
$T = 298$ (2) K
Block, green
0.23 × 0.19 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.887$, $T_{max} = 0.938$
24141 measured reflections

5091 independent reflections
4276 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 28.3°$
$h = -16 \rightarrow 16$
$k = -11 \rightarrow 11$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.107$
$S = 1.04$
5091 reflections
277 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2 + 0.452P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	2.011 (2)	Ni1—O8	2.127 (2)
Ni1—N2	2.079 (2)		
O1—Ni1—O1^i	180	N2—Ni1—O8^i	88.45 (5)
O1—Ni1—N2^i	91.46 (5)	O1—Ni1—O8	93.68 (5)
O1—Ni1—N2	88.54 (5)	N2—Ni1—O8	91.55 (5)
N2^i—Ni1—N2	180	O8^i—Ni1—O8	180
O1—Ni1—O8^i	86.32 (5)		

Symmetry code: (i) $-x + 1, -y + 2, -z + 2$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7B···O3^{ii}	0.83 (1)	2.60 (2)	3.250 (3)	136 (2)
O7—H7B···O2^{ii}	0.83 (1)	2.19 (1)	3.010 (2)	171 (3)
O7—H7A···O4	0.84 (1)	2.01 (1)	2.821 (3)	164 (3)
O8—H8···O7^{iii}	0.83 (1)	1.81 (1)	2.628 (2)	166 (3)
N3—H3B···O1^i	0.90	1.95	2.851 (2)	175
N3—H3A···N4^{iv}	0.90	2.58	3.454 (2)	163
N3—H3A···O5^{iv}	0.90	2.52	3.223 (2)	136
N3—H3A···O4^{iv}	0.90	1.95	2.839 (2)	167

Symmetry codes: (i) $-x + 1, -y + 2, -z + 2$; (ii) $x - 1, -y + \frac{3}{2}, z - \frac{1}{2}$; (iii) $x, -y + \frac{3}{2}, z + \frac{1}{2}$; (iv) $x, -y + \frac{5}{2}, z + \frac{1}{2}$.

Atoms H7*A*, H7*B* and H8 were located in a difference Fourier map and refined isotropically, with O—H and H···H distances restrained to 0.84 (1) and 1.37 (2) Å, respectively. All other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, N—H distances of 0.90 Å, and with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C/N)$. The U^{ij} components of atom O6 were restrained to isotropic behaviour.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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